

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016699.D
 Acq On : 03 Oct 2021 09:24
 Operator : CG/JU
 Sample : M3892-20
 Misc :
 ALS Vial : 67 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-832-J-SO-3-3.5-092221

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016699.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	10.457	735	737	740	rVB	254290	404930	1.03%	0.146%
2	12.074	939	947	969	rVB	295019	463034	1.18%	0.167%
3	12.296	986	997	1021	rBV	257438	406922	1.03%	0.147%
4	14.332	1185	1188	1191	rBV	3328872	4978267	12.65%	1.796%
5	15.321	1263	1266	1269	rBV	3694112	5860659	14.90%	2.114%
6	15.448	1271	1276	1277	rBV	330229	705765	1.79%	0.255%
7	15.486	1277	1279	1281	rVB	419083	576063	1.46%	0.208%
8	15.626	1288	1290	1294	rVB2	441852	674838	1.72%	0.243%
9	15.766	1299	1301	1305	rVB	455594	948834	2.41%	0.342%
10	16.323	1344	1346	1349	rVB	358630	648326	1.65%	0.234%
11	16.774	1379	1383	1386	rBV	600912	1106818	2.81%	0.399%
12	17.090	1404	1409	1411	rBV	12268047	26572154	67.55%	9.586%
13	17.163	1411	1415	1418	rVV	7267716	11018768	28.01%	3.975%
14	17.224	1418	1420	1423	rVB	361480	564617	1.44%	0.204%
15	17.431	1431	1437	1440	rBV2	1380197	2375828	6.04%	0.857%
16	17.906	1471	1476	1478	rBV	318579	558494	1.42%	0.201%
17	17.954	1478	1480	1483	rVB	474944	679141	1.73%	0.245%
18	18.422	1560	1567	1573	rBV	1234808	1675633	4.26%	0.604%
19	19.127	1697	1709	1714	rBV2	17179493	39339711	100.00%	14.192%
20	19.207	1721	1725	1731	rVB	441223	589095	1.50%	0.213%
21	19.341	1748	1752	1755	rVV2	302702	461059	1.17%	0.166%
22	19.370	1755	1758	1769	rVB2	279600	569041	1.45%	0.205%
23	19.489	1769	1782	1789	rBV3	16449614	38064072	96.76%	13.732%
24	19.539	1789	1792	1802	rVB	256405	420647	1.07%	0.152%
25	19.713	1822	1827	1834	rVB	1199118	1830299	4.65%	0.660%
26	19.926	1859	1870	1875	rBV3	198847	452283	1.15%	0.163%
27	20.027	1885	1888	1890	rBV2	216043	489717	1.24%	0.177%
28	20.123	1894	1897	1899	rBV3	325807	661773	1.68%	0.239%
29	20.165	1899	1901	1903	rVB	440519	533729	1.36%	0.193%
30	20.324	1910	1916	1920	rVB2	188952	484517	1.23%	0.175%
31	20.611	1940	1943	1944	rBV	487214	716092	1.82%	0.258%
32	20.685	1947	1950	1951	rBV	293526	498337	1.27%	0.180%
33	20.717	1951	1953	1957	rVB2	288096	611314	1.55%	0.221%
34	20.887	1965	1969	1971	rBV3	539138	1252514	3.18%	0.452%
35	20.930	1971	1973	1974	rVV	2554158	3046447	7.74%	1.099%
36	20.972	1974	1977	1980	rVV2	2092314	4358094	11.08%	1.572%

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Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 1 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.121	1988	1991	1993	rBV3	214248	462802	1.18%	0.167%
38	21.174	1993	1996	1997	rBV	509967	679985	1.73%	0.245%
39	21.238	1997	2002	2004	rVV	10955078	21832405	55.50%	7.876%
40	21.291	2004	2007	2010	rVB	10703210	19461372	49.47%	7.021%
41	21.408	2015	2018	2021	rBV	3193731	4881181	12.41%	1.761%
42	21.801	2051	2055	2057	rVB2	403672	715281	1.82%	0.258%
43	21.960	2064	2070	2072	rBV3	730506	2124398	5.40%	0.766%
44	22.002	2072	2074	2075	rVV2	774833	1139349	2.90%	0.411%
45	22.034	2075	2077	2080	rVB	1427611	1991991	5.06%	0.719%
46	22.109	2080	2084	2088	rVB2	670399	1273285	3.24%	0.459%
47	22.278	2097	2100	2104	rBV2	350218	865402	2.20%	0.312%
48	22.584	2155	2164	2180	rVB	540269	926849	2.36%	0.334%
49	22.752	2205	2213	2223	rBV	308526	553192	1.41%	0.200%
50	22.847	2224	2241	2249	rBV	6312167	18282835	46.47%	6.596%
51	23.008	2278	2288	2299	rVB	1750139	2940128	7.47%	1.061%
52	23.327	2368	2381	2396	rBV	4038072	8997595	22.87%	3.246%
53	23.429	2396	2411	2426	rVB	5606107	12229158	31.09%	4.412%
54	23.566	2440	2451	2464	rVB	2041230	4065810	10.34%	1.467%
55	24.395	2683	2693	2715	rVB	327655	745083	1.89%	0.269%
56	25.206	2917	2930	2943	rVV5	136925	405996	1.03%	0.146%
57	25.504	3004	3017	3026	rBV2	445809	1247416	3.17%	0.450%
58	25.812	3090	3107	3126	rVB2	2362781	6967803	17.71%	2.514%
59	25.925	3128	3140	3166	rVB2	255291	801006	2.04%	0.289%
60	26.079	3169	3185	3198	rBV	512021	1434808	3.65%	0.518%
61	26.168	3199	3211	3224	rBV2	347294	937360	2.38%	0.338%
62	26.513	3290	3312	3340	rBV2	1458159	5091897	12.94%	1.837%
63	26.876	3401	3418	3455	rVB	460787	1548838	3.94%	0.559%

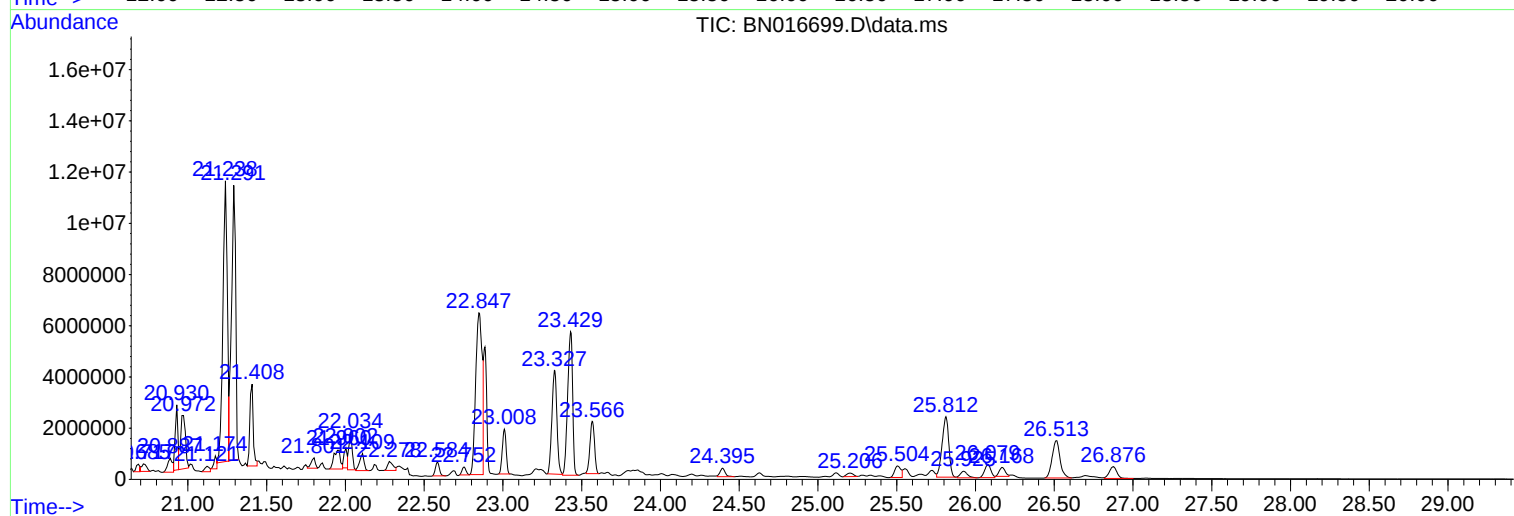
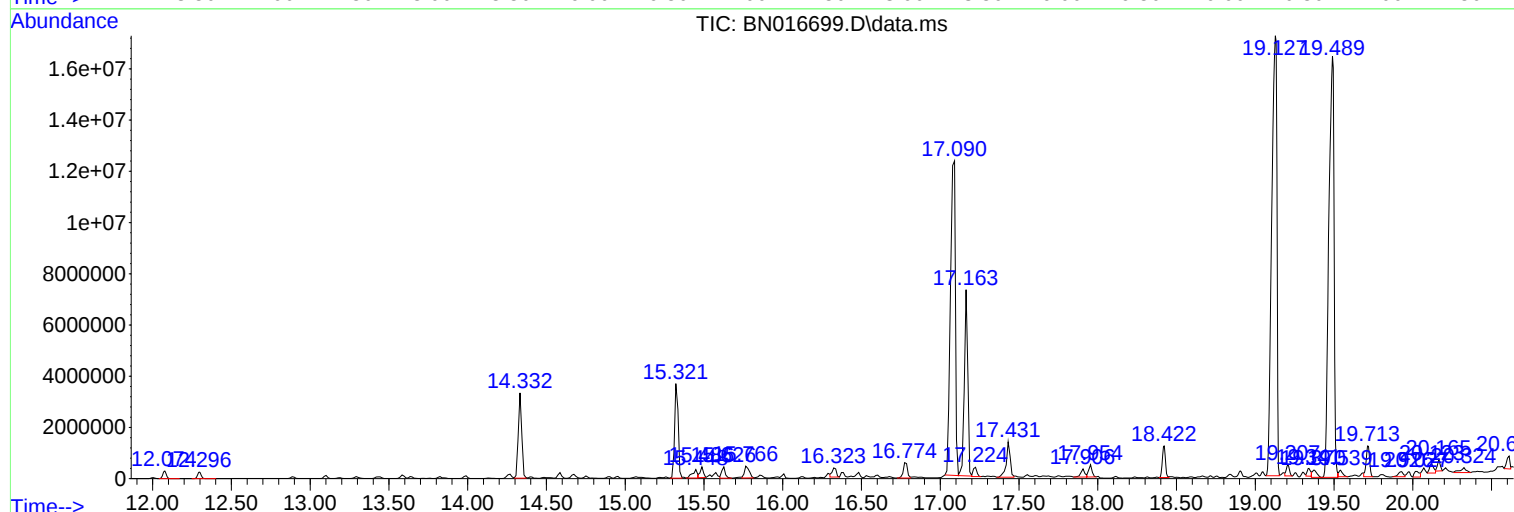
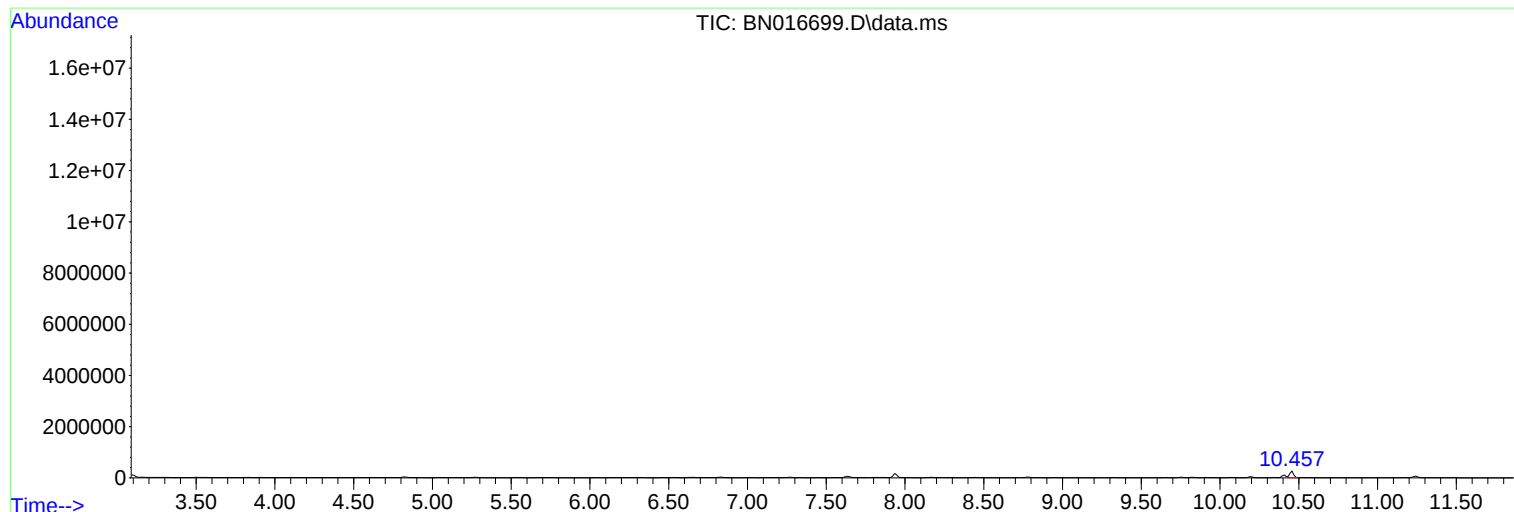
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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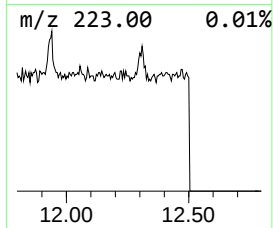
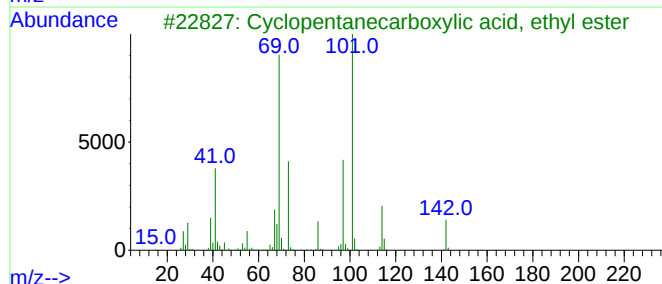
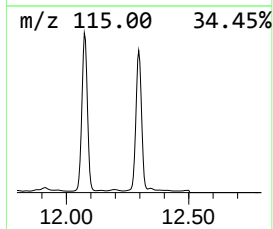
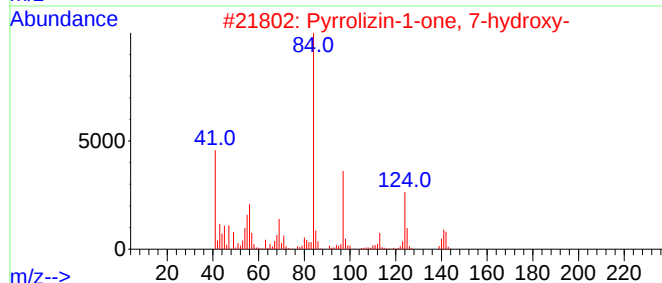
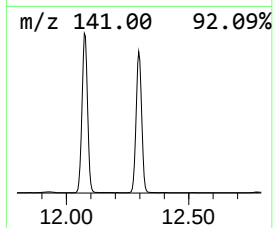
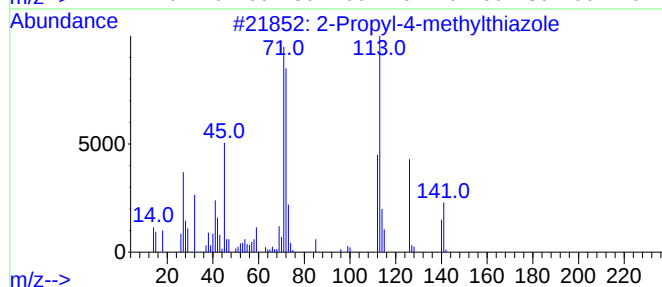
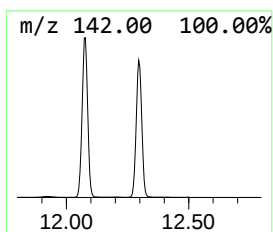
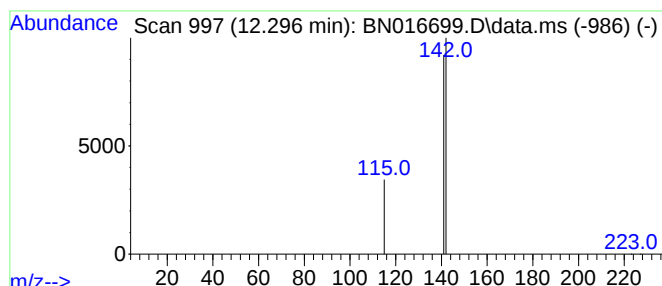
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Propyl-4-methylthiazole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.296	0.40 ng	406922	Naphthalene-d8	10.406

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2		Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3		Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4		2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5		2,4(1H,3H)-Pyrimidinedione, 6-am...	141	C5H7N3O2	002434-53-9	2



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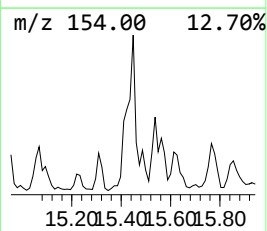
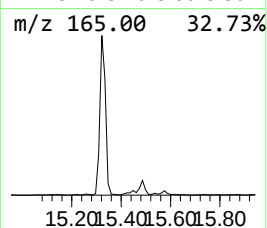
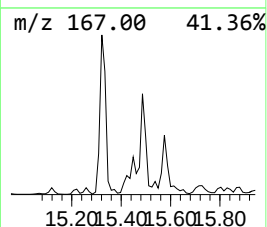
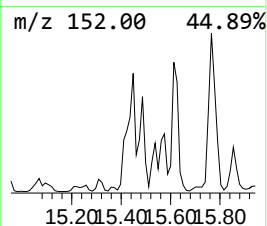
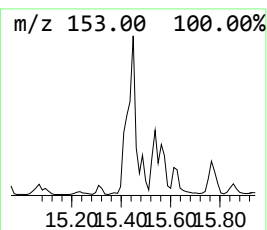
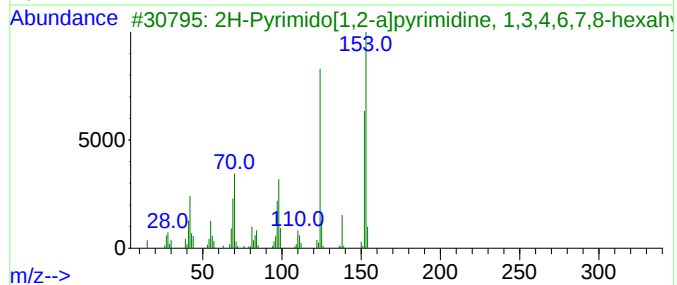
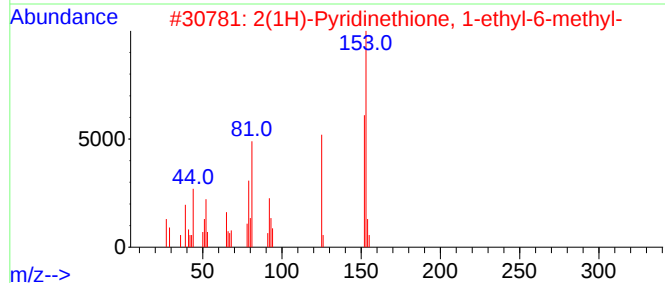
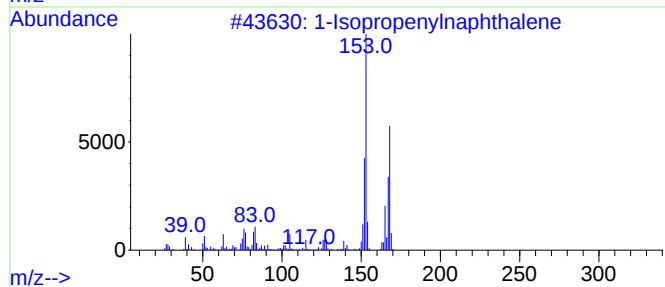
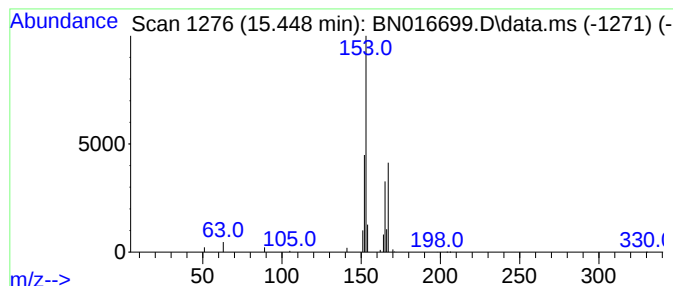
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Isopropenylnaphthalene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.448	0.06 ng	705765	Acenaphthene-d10	14.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Isopropenylnaphthalene	168	C13H12	001855-47-6	56
2			2(1H)-Pyridinethione, 1-ethyl-6-...	153	C8H11NS	019006-73-6	9
3			2H-Pyrimido[1,2-a]pyrimidine, 1,...	153	C8H15N3	084030-20-6	9
4			Benzeneacetonitrile, 2,6-difluoro-	153	C8H5F2N	000654-01-3	9
5			3-Pyridinemethanol, 5-hydroxy-4,...	153	C8H11NO2	000061-67-6	9



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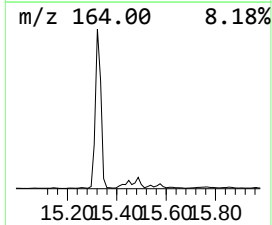
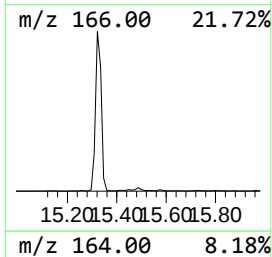
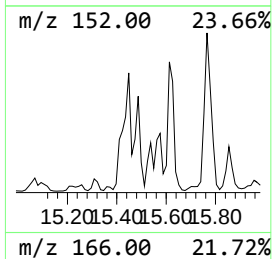
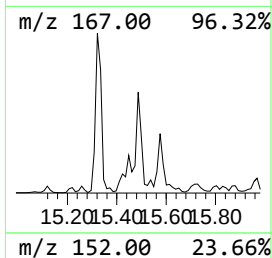
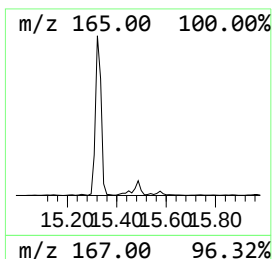
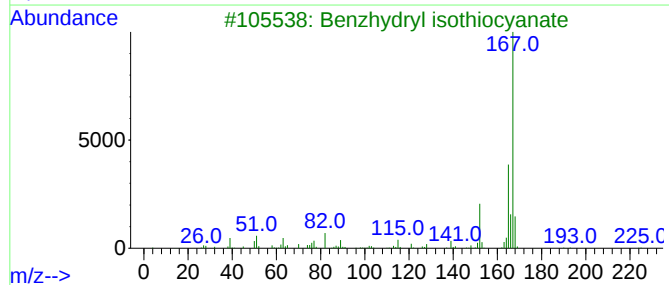
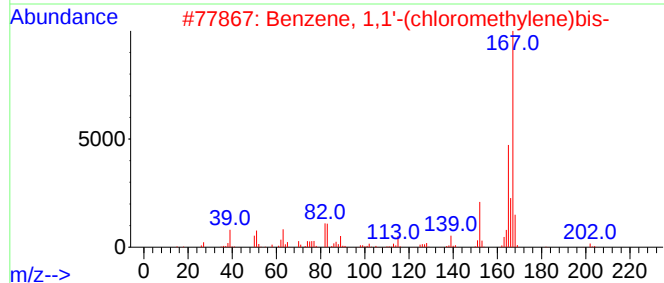
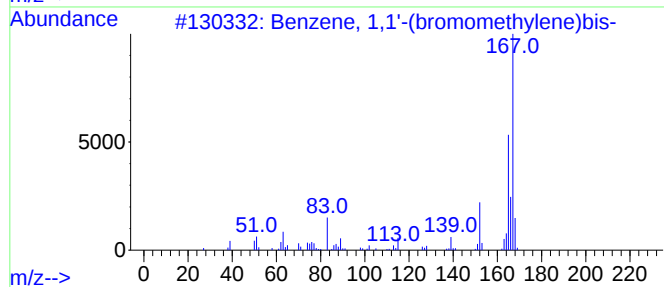
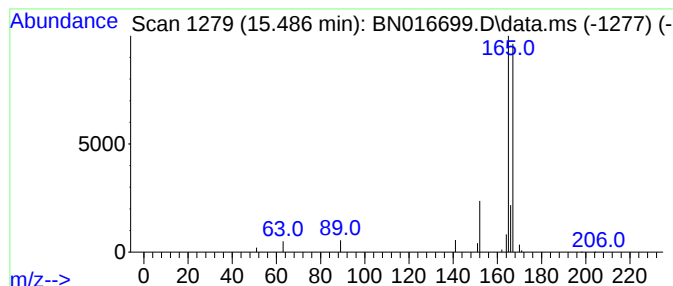
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,1'-(bromomethyle... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	0.05 ng	576063	Acenaphthene-d10	14.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(bromomethylene)bis-	246	C13H11Br	000776-74-9	59
2			Benzene, 1,1'-(chloromethylene)bis-	202	C13H11Cl	000090-99-3	59
3			Benzhydryl isothiocyanate	225	C14H11NS	003550-21-8	40
4			2-Propanone, 1,1-diphenyl-	210	C15H14O	000781-35-1	12
5			Cyclohexane-1,3-dione, 2-dimethy...	167	C9H13NO2	085302-07-4	9



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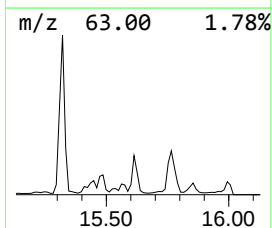
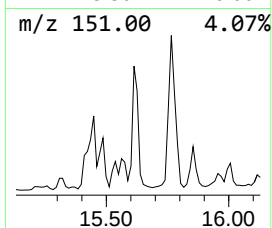
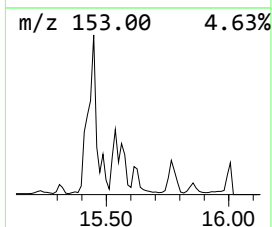
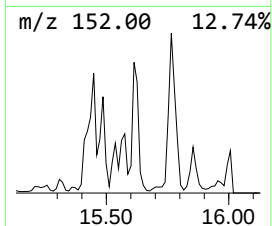
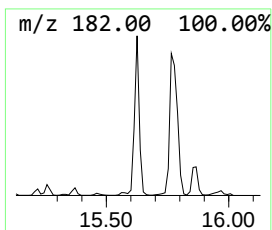
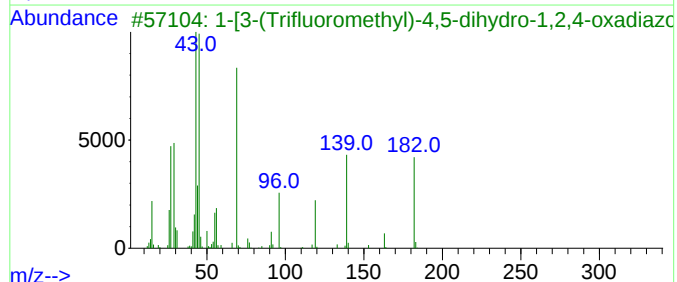
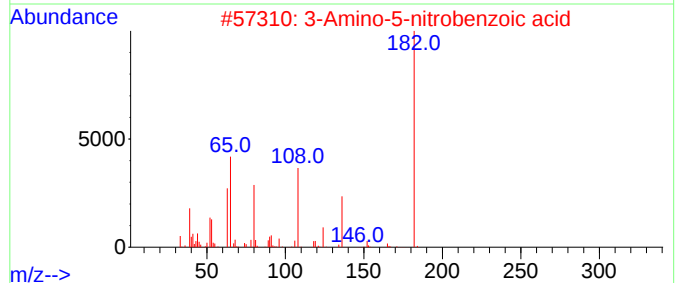
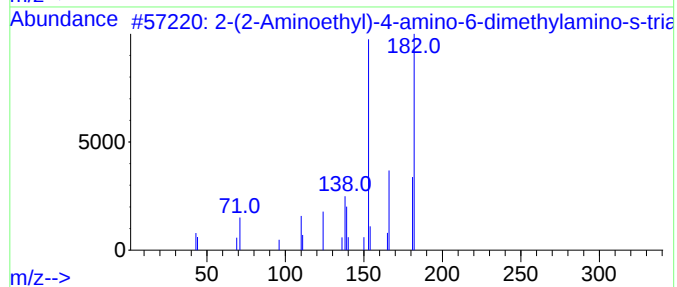
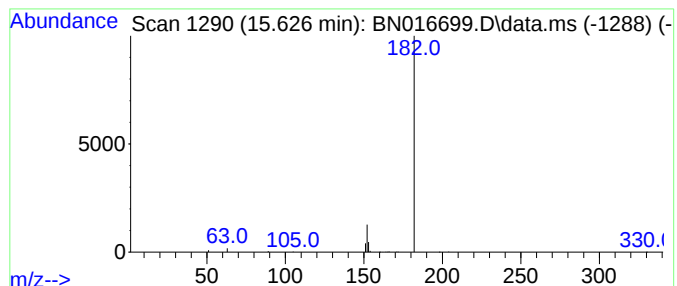
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-(2-Aminoethyl)-4-amino-6-... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.626	0.05 ng	674838	Acenaphthene-d10	14.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Aminoethyl)-4-amino-6-dimet...	182	C7H14N6	040917-13-3	2		
2	3-Amino-5-nitrobenzoic acid	182	C7H6N2O4	000618-84-8	2		
3	1-[3-(Trifluoromethyl)-4,5-dihyd...	182	C5H5F3N2O2	1000443-70-5	2		
4	Ethyl 4-hydroxy-2-methyl-5-pyrim...	182	C8H10N2O3	053135-24-3	2		
5	1,3-Benzenediol, 0-methoxyacetyl-	182	C9H10O4	1010345-49-2	2		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
Acq On : 03 Oct 2021 09:24
Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-3-3.5-092221

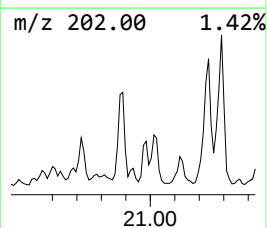
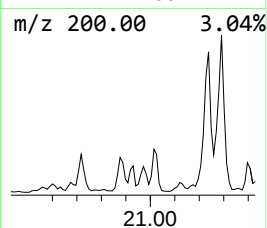
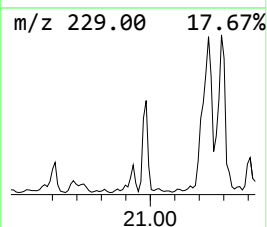
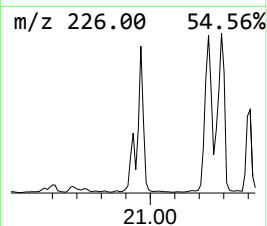
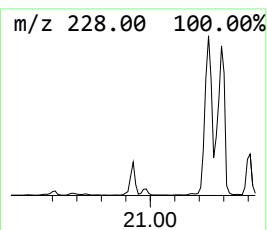
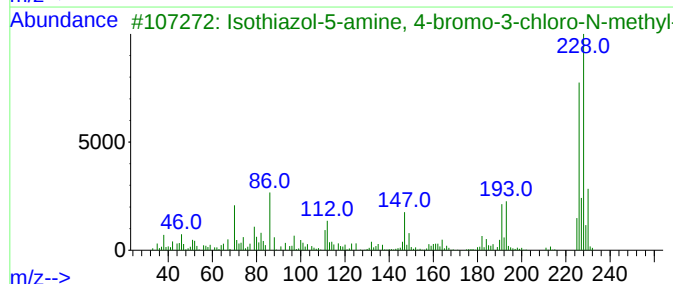
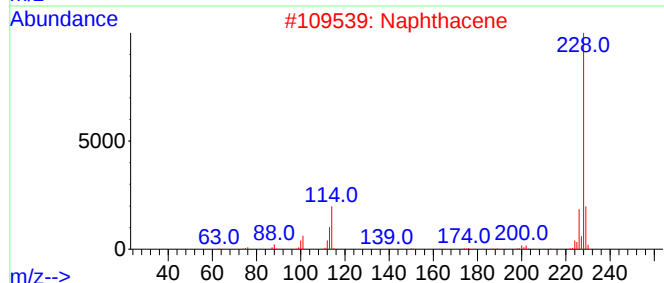
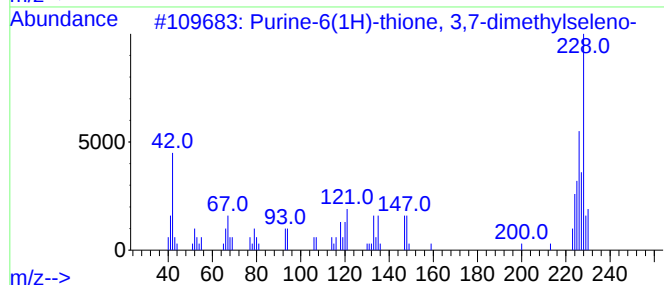
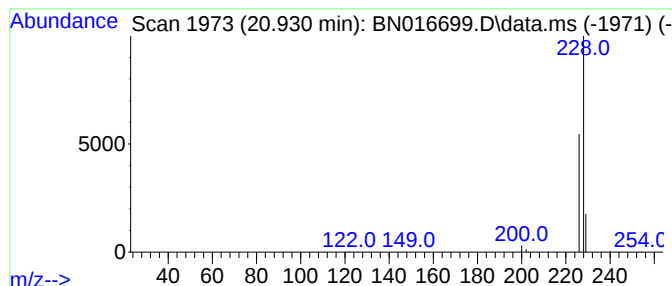
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Purine-6(1H)-thione, 3,7-di... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.930	0.06 ng	3046450	Chrysene-d12	21.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Purine-6(1H)-thione, 3,7-dimethy...	228	C7H8N4Se	023663-58-3	64
2			Naphthacene	228	C18H12	000092-24-0	40
3			Isothiazol-5-amine, 4-bromo-3-ch...	226	C4H4BrClN2S	1000272-59-9	9
4			Chrysene	228	C18H12	000218-01-9	9
5			Benz[a]anthracene	228	C18H12	000056-55-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
Acq On : 03 Oct 2021 09:24
Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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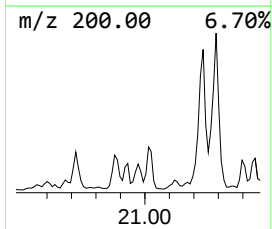
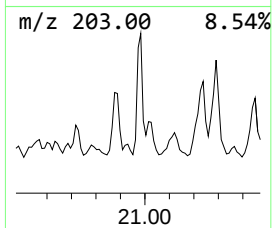
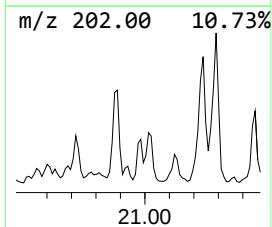
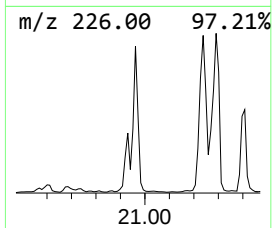
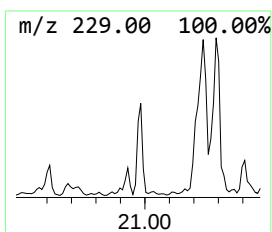
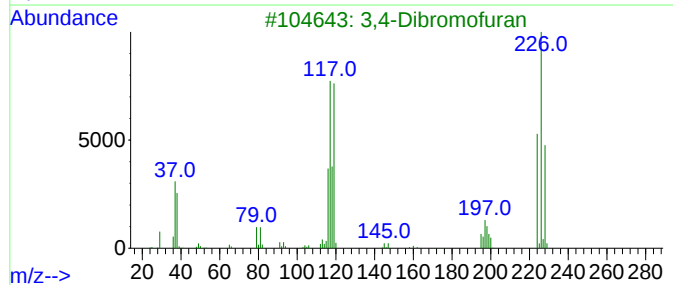
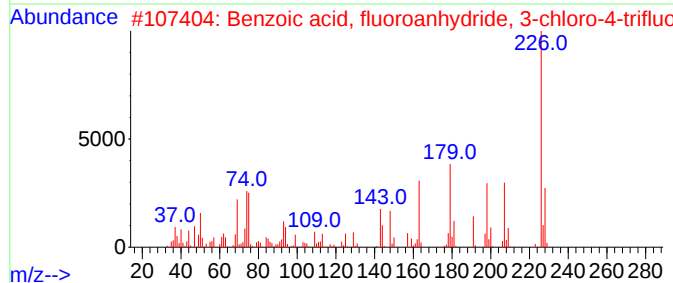
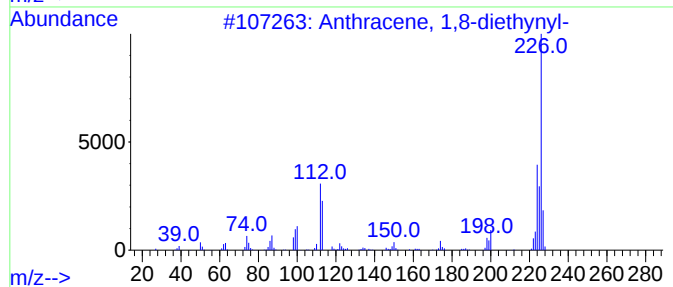
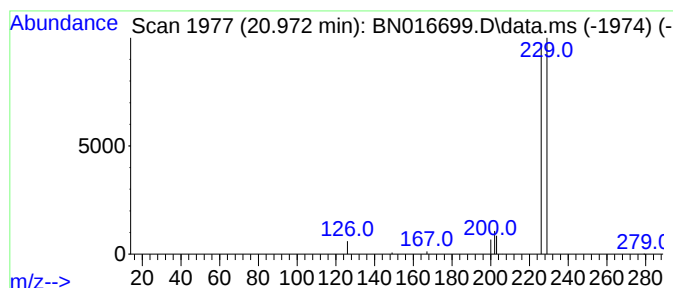
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Anthracene, 1,8-diethynyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.972	0.08 ng	4358090	Chrysene-d12	21.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1,8-diethynyl-	226	C18H10	078053-58-4	4
2			Benzoic acid, fluoroanhydride, 3...	226	C8H3ClF4O	000320-62-7	4
3			3,4-Dibromofuran	224	C4H2Br2O	032460-02-9	4
4			9H-Xanthen-9-one, 2-methoxy-	226	C14H10O3	001214-20-6	4
5			Benzene, [4-(3-ethynylphenyl)-1,...	226	C18H10	1000115-87-3	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
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Sample : M3892-20
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ALS Vial : 67 Sample Multiplier: 1

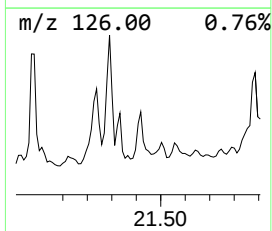
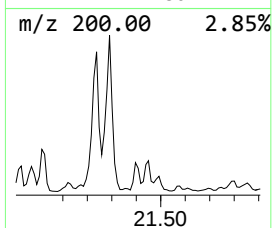
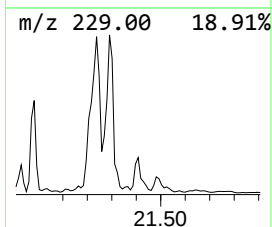
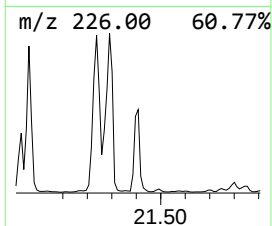
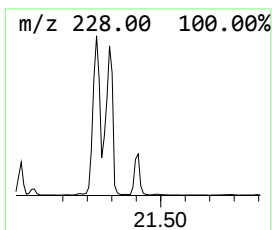
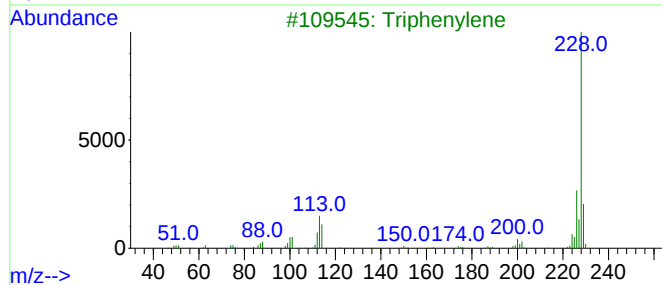
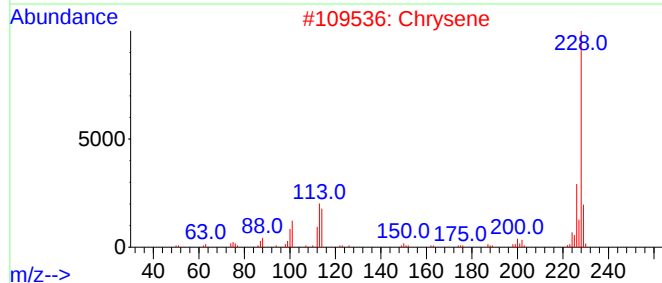
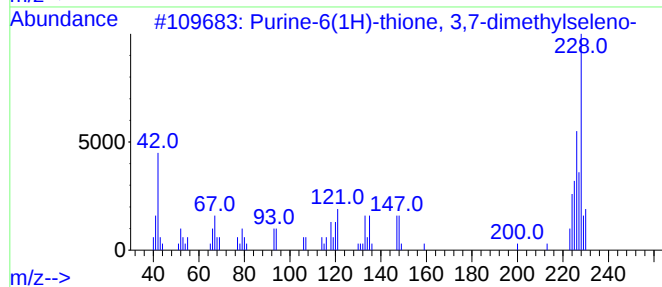
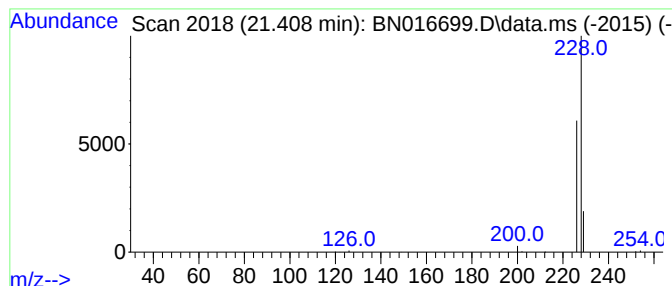
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Purine-6(1H)-thione, 3,7-di... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.408	0.09 ng	4881180	Chrysene-d12	21.259	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Purine-6(1H)-thione, 3,7-dimethy...	228	C7H8N4Se	023663-58-3	64
2	Chrysene	228	C18H12	000218-01-9	9
3	Triphenylene	228	C18H12	000217-59-4	9
4	Naphthacene	228	C18H12	000092-24-0	9
5	Benzo[c]phenanthrene	228	C18H12	000195-19-7	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
Acq On : 03 Oct 2021 09:24
Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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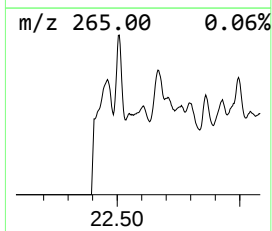
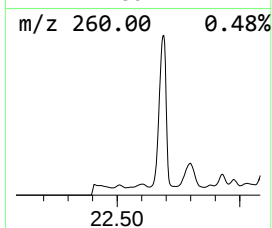
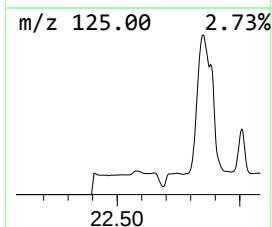
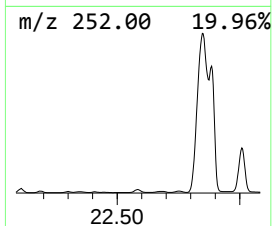
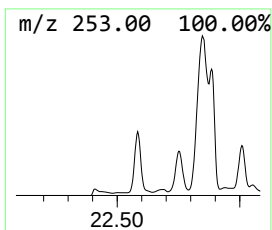
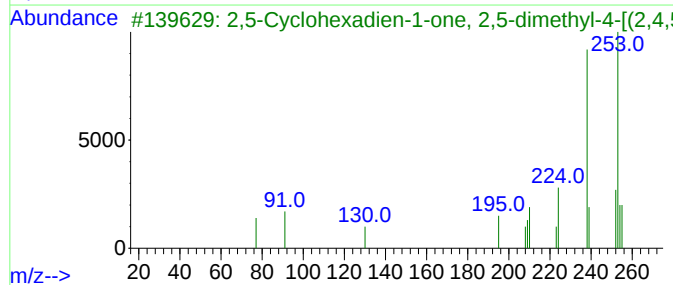
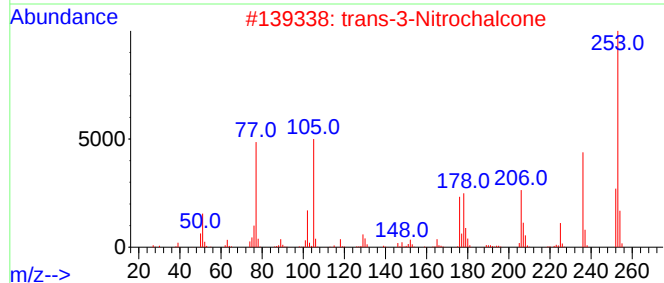
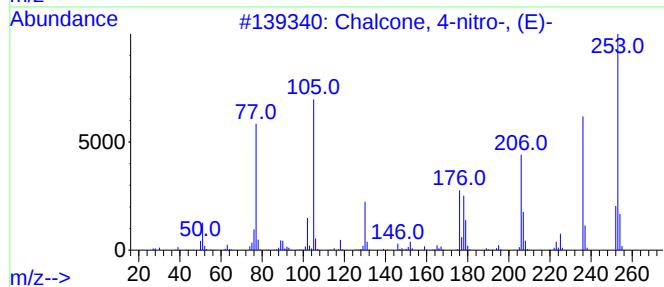
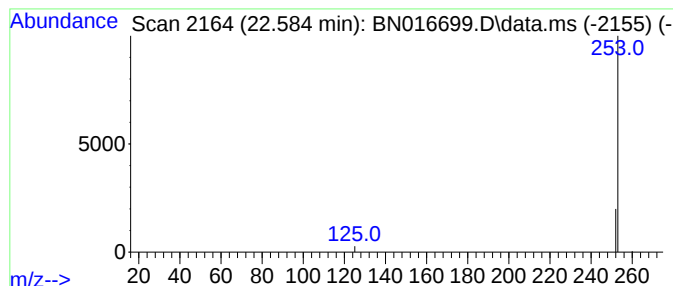
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Chalcone, 4-nitro-, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.584	0.09 ng	926849	Perylene-d12	23.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chalcone, 4-nitro-, (E)-	253	C15H11NO3	002960-55-6	5
2			trans-3-Nitrochalcone	253	C15H11NO3	024721-24-2	5
3			2,5-Cyclohexadien-1-one, 2,5-dimethyl-4-[(2,4,6-trimethylphenyl)imino]-	253	C17H19NO	054245-93-1	5
4			Pyrimidine, 4-methyl-2-phenyl-6-(1H-imidazol-2-yl)-	253	C16H19N3	1000302-39-3	5
5			1-(4-Fluorophenyl)-3-phenyl-1H-pyrazole	253	C15H12FN3	072411-51-9	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
Acq On : 03 Oct 2021 09:24
Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
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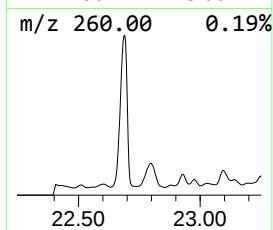
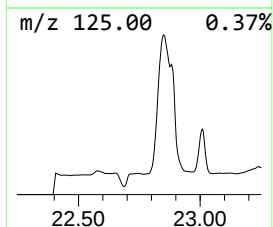
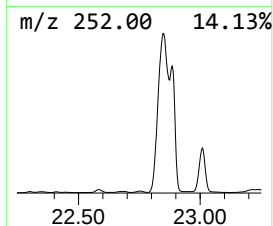
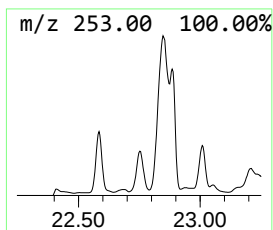
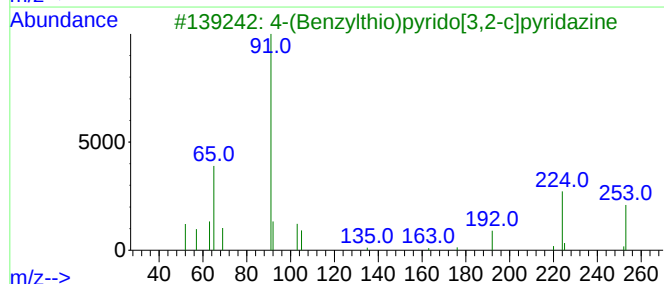
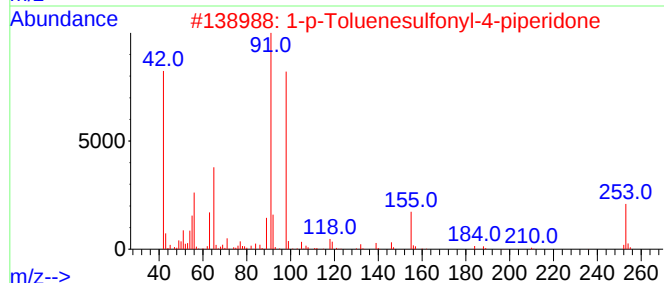
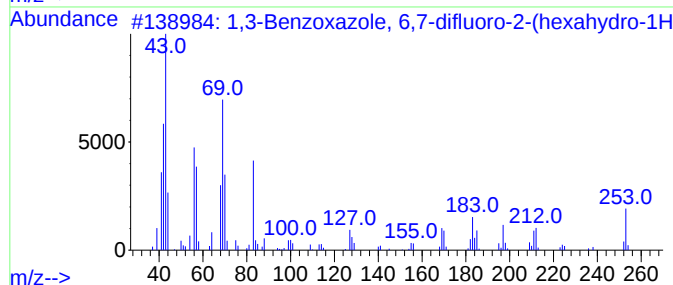
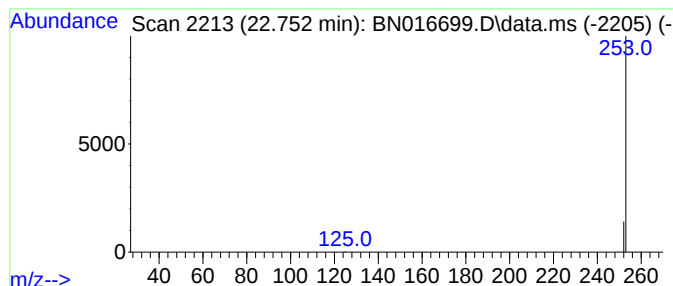
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1,3-Benzoxazole, 6,7-difluo... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.752	0.05 ng	553192	Perylene-d12	23.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzoxazole, 6,7-difluoro-2-...	253	C12H13F2N3O	1000362-81-2	4		
2	1-p-Toluenesulfonyl-4-piperidone	253	C12H15NO3S	033439-27-9	4		
3	4-(Benzylthio)pyrido[3,2-c]pyrid...	253	C14H11N3S	1000326-92-1	3		
4	Thiophene-2-carboxamide, N-ethyl...	253	C14H23NOS	1000415-31-0	3		
5	p-Toluyamide, N-(2-phenylethyl)...	253	C17H19NO	1010451-68-2	3		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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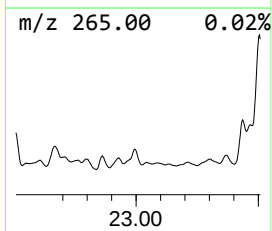
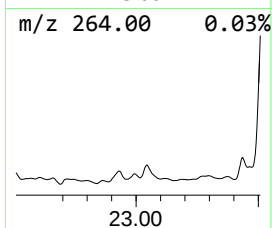
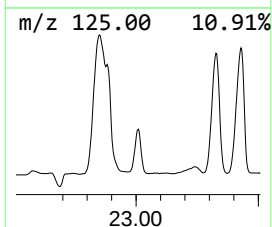
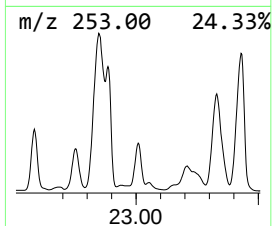
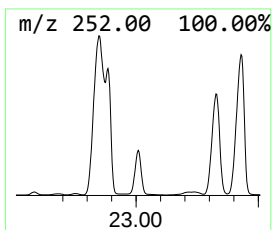
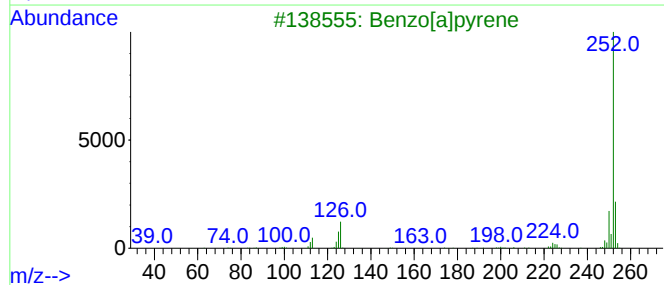
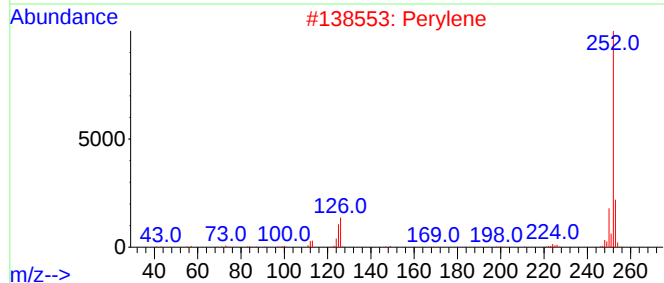
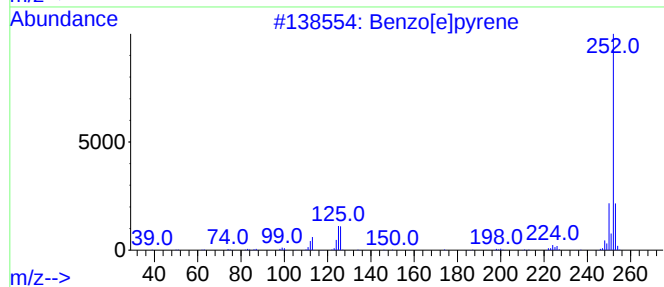
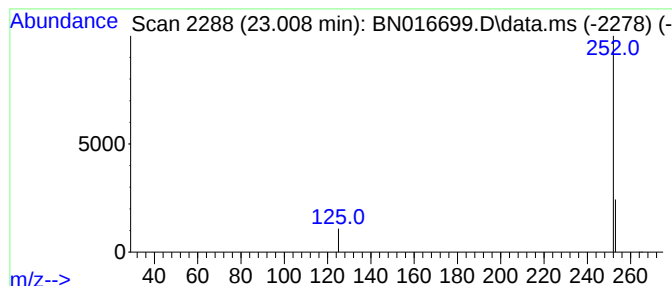
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.008	0.29 ng	2940130	Perylene-d12	23.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	9
2			Perylene	252	C20H12	000198-55-0	9
3			Benzo[a]pyrene	252	C20H12	000050-32-8	9
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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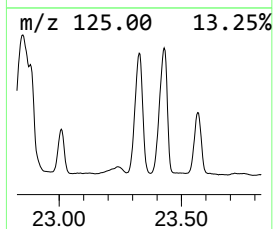
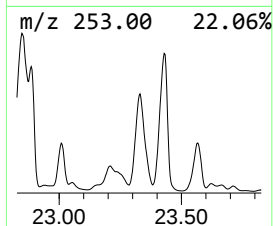
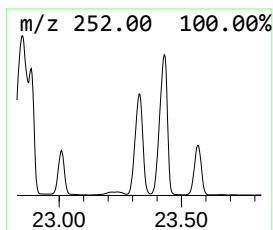
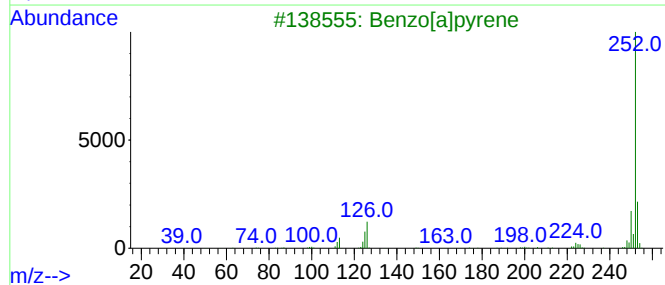
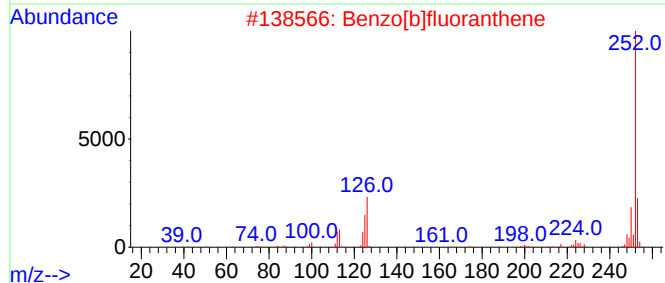
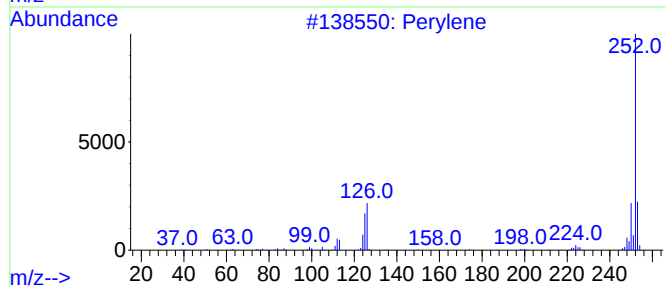
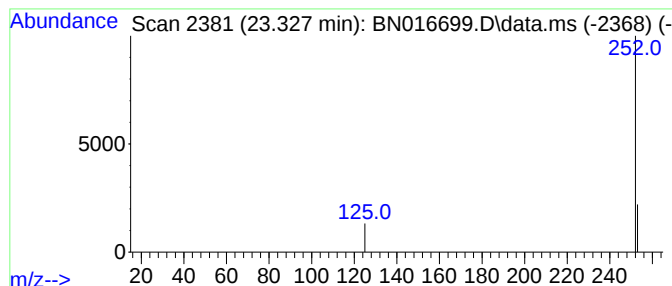
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.327	0.89 ng	8997600	Perylene-d12	23.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	9
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
3			Benzo[a]pyrene	252	C20H12	000050-32-8	9
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	9
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
Acq On : 03 Oct 2021 09:24
Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

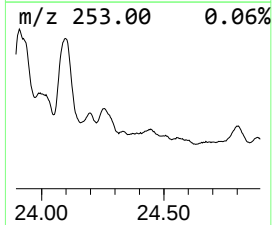
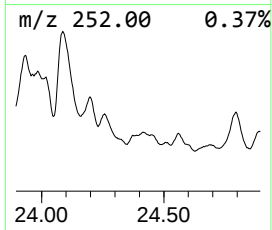
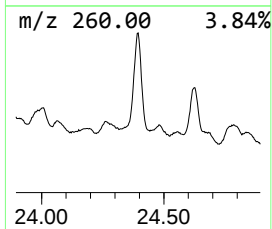
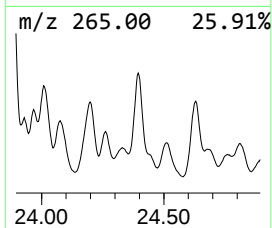
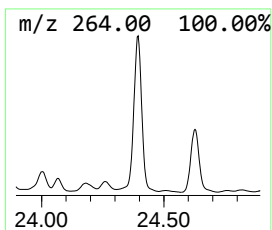
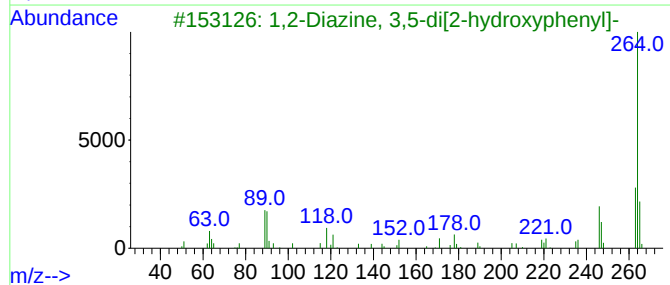
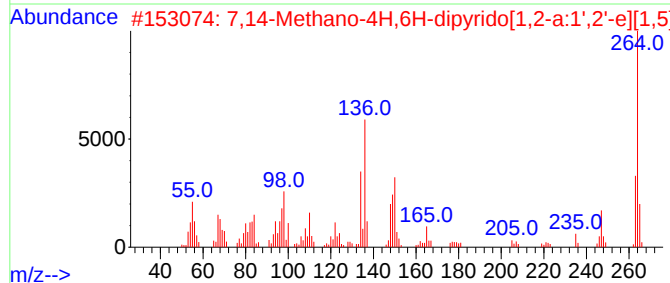
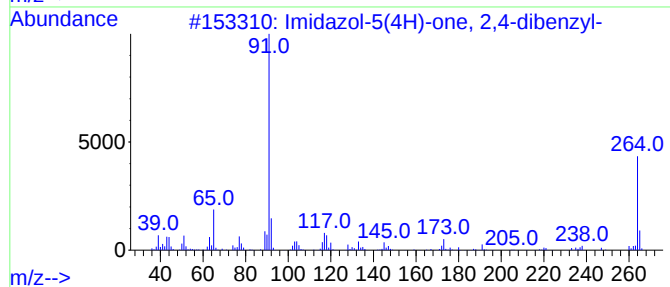
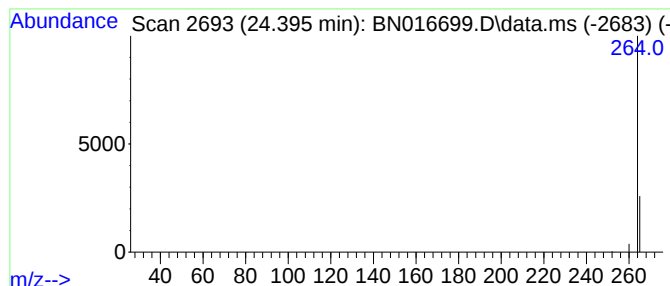
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ClientSampleId :
S-832-J-SO-3-3.5-092221

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Imidazol-5(4H)-one, 2,4-dib... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.395	0.07 ng	745083	Perylene-d12	23.518	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazol-5(4H)-one, 2,4-dibenzyl-	264	C17H16N2O	097978-58-0	9
2	7,14-Methano-4H,6H-dipyrido[1,2-...	264	C15H24N2O2	023360-87-4	5
3	1,2-Diazine, 3,5-di[2-hydroxyphe...	264	C16H12N2O2	122763-54-6	5
4	Chrysene-1,7(2H,8H)-dione, 3,4,9...	264	C18H16O2	039500-23-7	5
5	4-Methylimidazole-5-diphenylmeth...	264	C17H16N2O	086347-08-2	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
Acq On : 03 Oct 2021 09:24
Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-3-3.5-092221

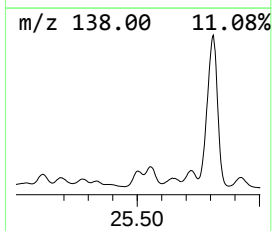
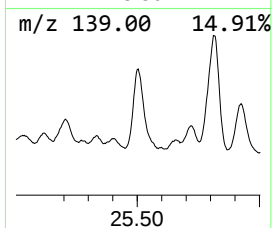
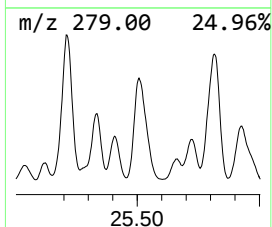
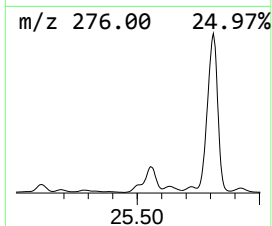
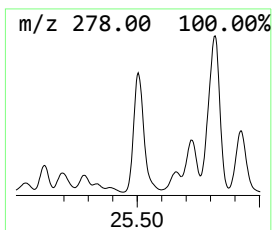
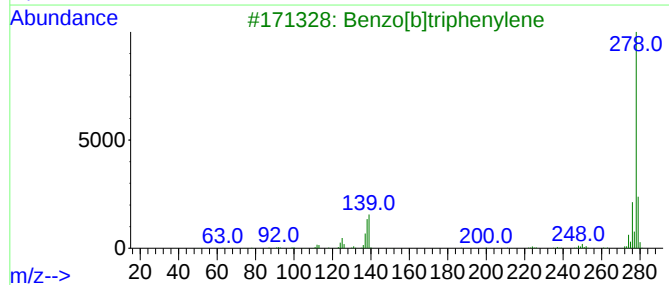
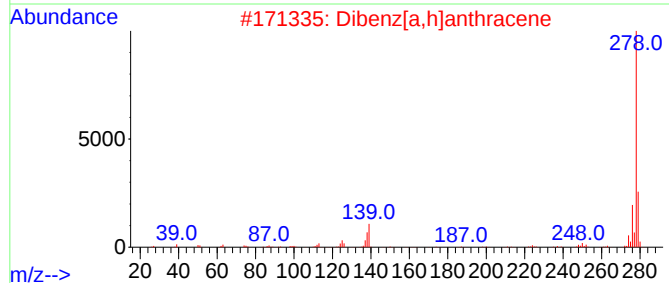
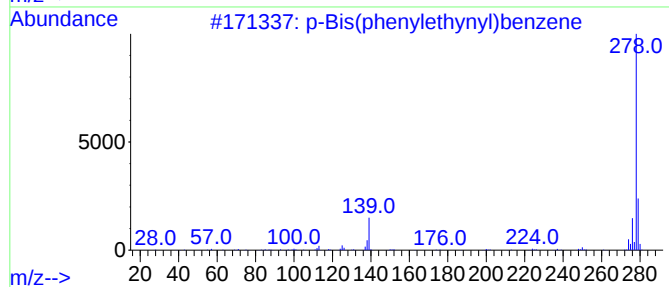
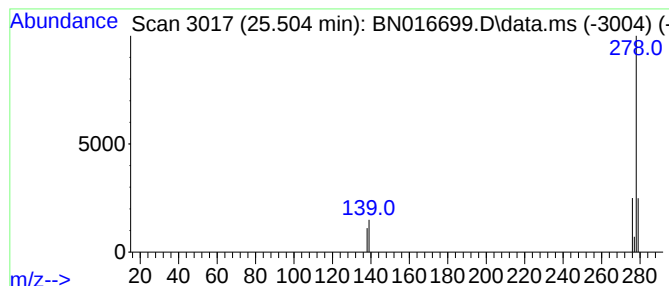
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 p-Bis(phenylethynyl)benzene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.504	0.12 ng	1247420	Perylene-d12	23.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Bis(phenylethynyl)benzene	278	C22H14	001849-27-0	72
2			Dibenz[a,h]anthracene	278	C22H14	000053-70-3	64
3			Benzo[b]triphenylene	278	C22H14	000215-58-7	64
4			Pentaphene	278	C22H14	000222-93-5	64
5			3-(3-Phenoxyphenoxy)phenol	278	C18H14O3	014200-84-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
Acq On : 03 Oct 2021 09:24
Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-3-3.5-092221

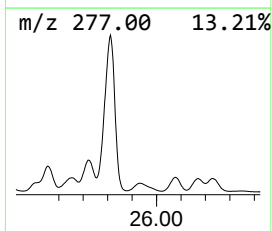
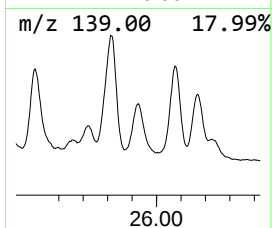
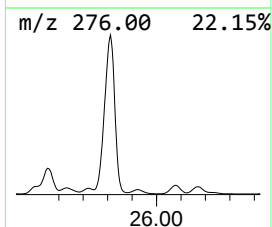
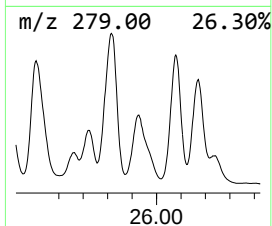
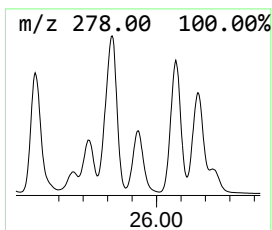
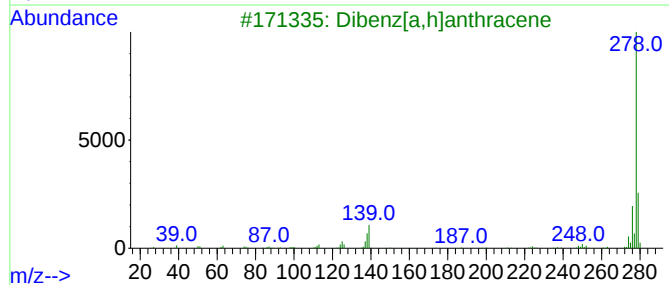
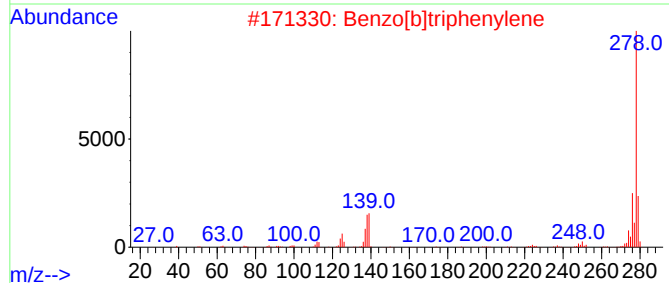
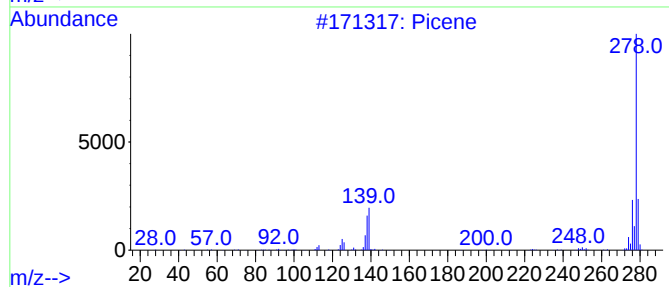
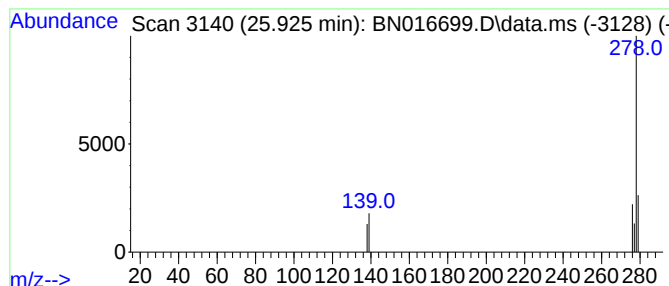
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Picene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.925	0.08 ng	801006	Perylene-d12	23.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Picene	278	C22H14	000213-46-7	80
2			Benzo[b]triphenylene	278	C22H14	000215-58-7	80
3			Dibenz[a,h]anthracene	278	C22H14	000053-70-3	72
4			1-naphthalenol, 4-[2-(4-methoxyp...	278	C17H14N2O2	1000397-12-8	56
5			1-(Diethylamino)-3-methylpyrido[...	278	C17H18N4	1000331-84-4	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
Acq On : 03 Oct 2021 09:24
Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-3-3.5-092221

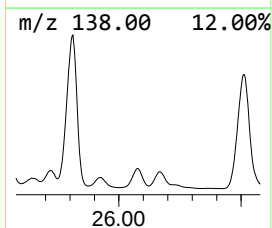
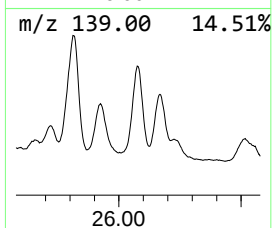
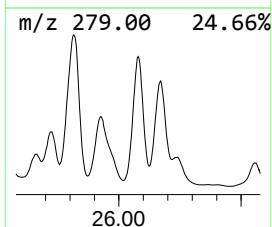
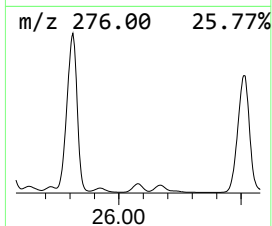
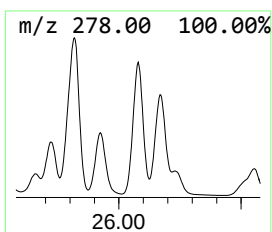
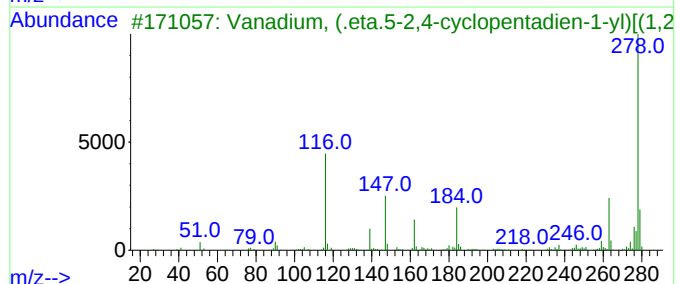
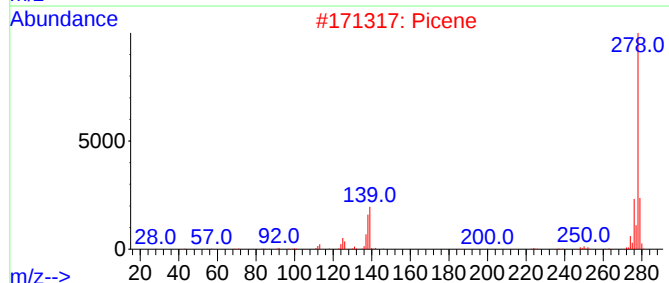
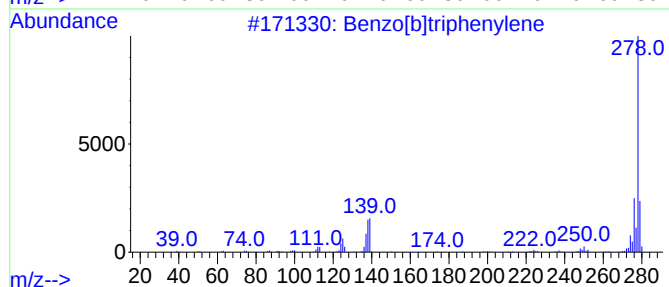
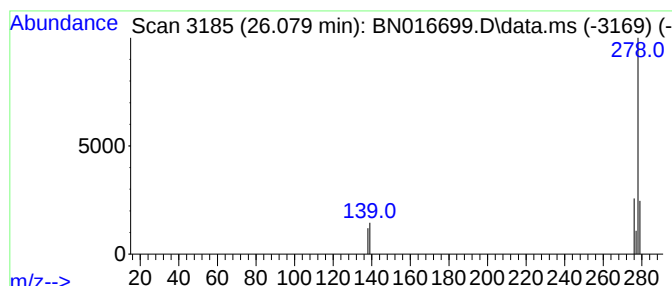
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Benzo[b]triphenylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.079	0.14 ng	1434810	Perylene-d12	23.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]triphenylene	278	C22H14	000215-58-7	80
2			Picene	278	C22H14	000213-46-7	80
3			Vanadium, (.eta.5-2,4-cyclopenta...	278	C17H23V	126948-97-8	78
4			Pentaphene	278	C22H14	000222-93-5	72
5			1-naphthalenol, 4-[2-(4-methoxyp...	278	C17H14N2O2	1000397-12-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
Acq On : 03 Oct 2021 09:24
Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-3-3.5-092221

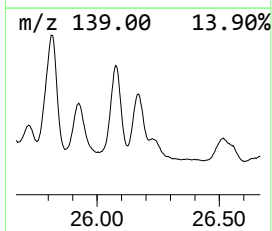
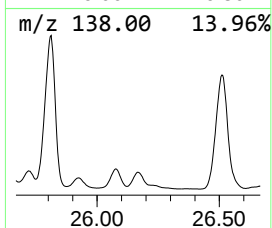
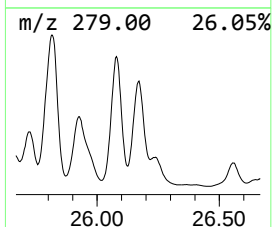
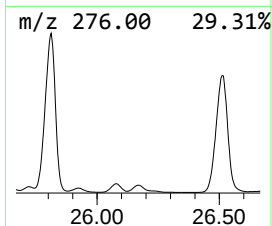
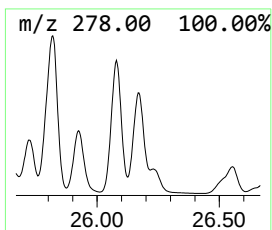
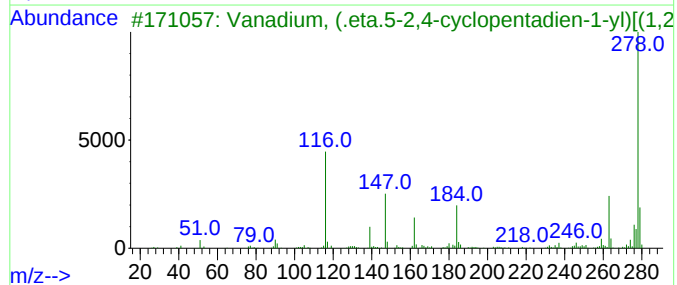
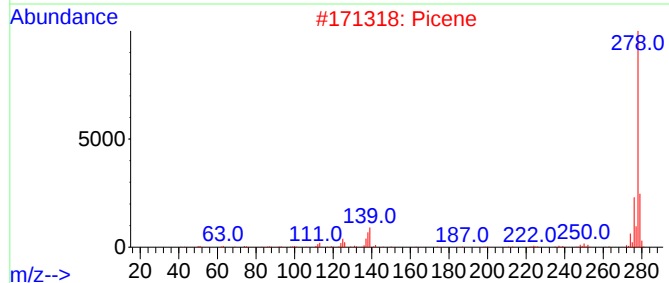
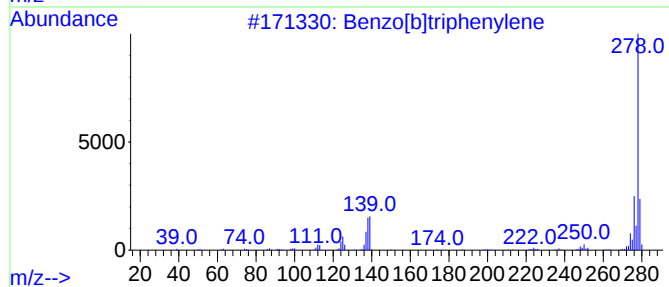
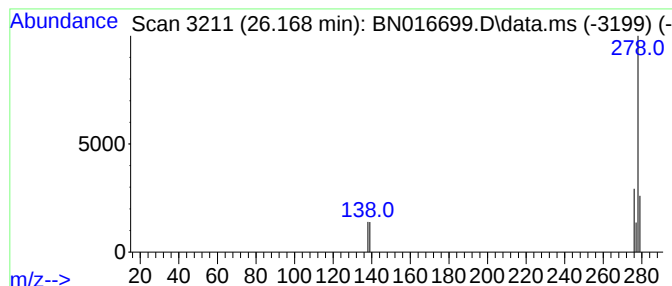
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Benzo[b]triphenylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.168	0.09 ng	937360	Perylene-d12	23.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]triphenylene	278	C22H14	000215-58-7	80
2			Picene	278	C22H14	000213-46-7	80
3			Vanadium, (.eta.5-2,4-cyclopenta...	278	C17H23V	126948-97-8	78
4			Benz[a]anthracene-7,12-dicarboni...	278	C20H10N2	035215-32-8	72
5			1-naphthalenol, 4-[2-(4-methoxy...	278	C17H14N2O2	1000397-12-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016699.D
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Operator : CG/JU
Sample : M3892-20
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-3-3.5-092221

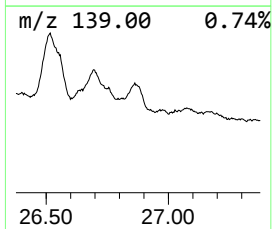
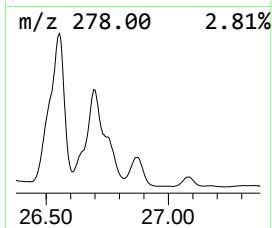
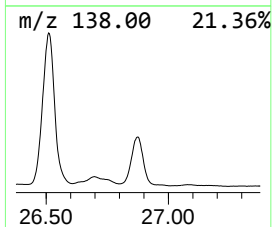
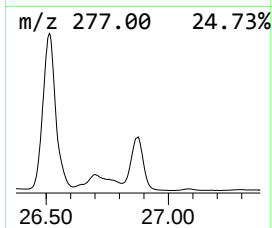
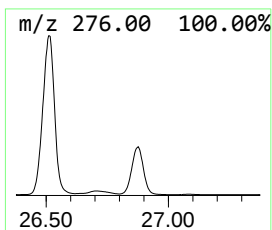
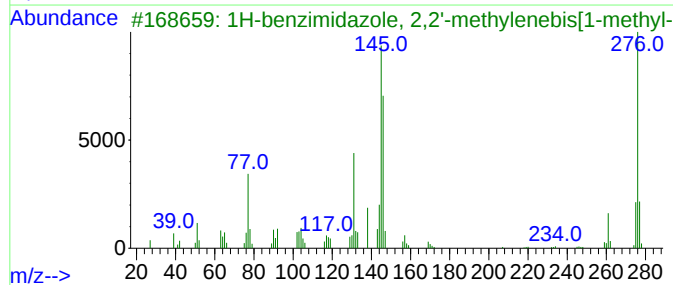
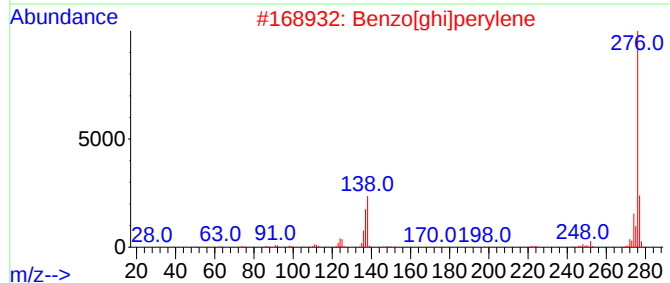
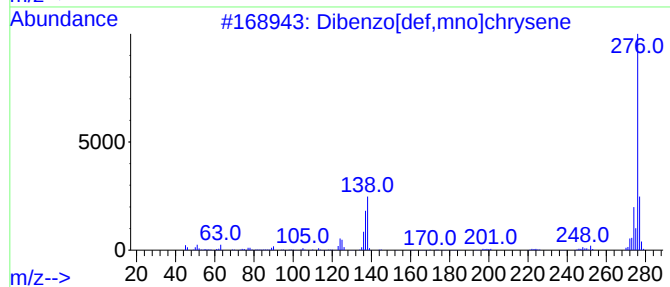
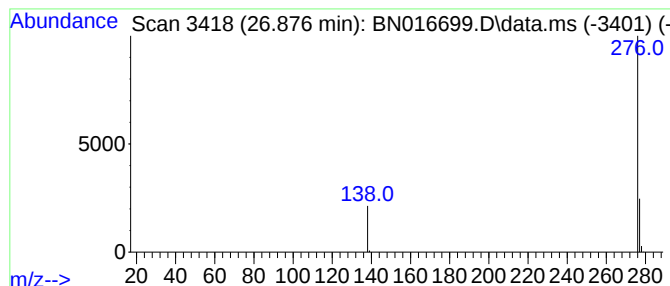
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Dibenzo[def,mno]chrysene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.876	0.15 ng	1548840	Perylene-d12	23.518

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	83
2			Benzo[ghi]perylene	276	C22H12	000191-24-2	83
3			1H-benzimidazole, 2,2'-methylene...	276	C17H16N4	1000401-82-9	83
4			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	83
5			2-Benzyloxazolo[4,5-c]quinolin-4...	276	C17H12N2O2	211874-80-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016699.D
 Acq On : 03 Oct 2021 09:24
 Operator : CG/JU
 Sample : M3892-20
 Misc :
 ALS Vial : 67 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-832-J-SO-3-3.5-092221

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propyl-4-meth...	12.296	0.4	ng	406922	2	10.406	404930	0.4
1-Isopropenylna...	15.448	0.1	ng	705765	3	14.268	4978270	0.4
Benzene, 1,1'-(...	15.486	0.0	ng	576063	3	14.268	4978270	0.4
2-(2-Aminoethyl...	15.626	0.1	ng	674838	3	14.268	4978270	0.4
Purine-6(1H)-th...	20.930	0.1	ng	3046450	5	21.259	21832400	0.4
Anthracene, 1,8...	20.972	0.1	ng	4358090	5	21.259	21832400	0.4
Purine-6(1H)-th...	21.408	0.1	ng	4881180	5	21.259	21832400	0.4
Chalcone, 4-nit...	22.584	0.1	ng	926849	6	23.518	4065810	0.4
1,3-Benzoxazole...	22.752	0.1	ng	553192	6	23.518	4065810	0.4
Benzo[e]pyrene	23.008	0.3	ng	2940130	6	23.518	4065810	0.4
Perylene	23.327	0.9	ng	8997600	6	23.518	4065810	0.4
Imidazol-5(4H)-...	24.395	0.1	ng	745083	6	23.518	4065810	0.4
p-Bis(phenyleth...	25.504	0.1	ng	1247420	6	23.518	4065810	0.4
Picene	25.925	0.1	ng	801006	6	23.518	4065810	0.4
Benzo[b]triphen...	26.079	0.1	ng	1434810	6	23.518	4065810	0.4
Benzo[b]triphen...	26.168	0.1	ng	937360	6	23.518	4065810	0.4
Dibenzo[def,mno...	26.876	0.2	ng	1548840	6	23.518	4065810	0.4